

# NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

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TECHNICAL REPORT  
R-81

## ALIGNMENT CHARTS FOR TRANSPORT PROPERTIES VISCOSITY, THERMAL CONDUCTIVITY, AND DIFFUSION COEFFICIENTS FOR NONPOLAR GASES AND GAS MIXTURES AT LOW DENSITY

By RICHARD S. BROKAW

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### SUMMARY

*In problems involving fluid flow, heat transfer, and mass transfer of gases, the viscosities, thermal conductivities, and diffusion coefficients are required. Direct measurements are in any event time consuming—they may be impossible.*

*Alignment charts (nomographs) for calculating the low-pressure transport properties of nonpolar gases and gas mixtures are presented. Calculations for pure gases are based on the rigorous kinetic theory of gases as applied to a realistic intermolecular force law. Mixture viscosities and conductivities are calculated from good approximations derived from rigorous theory.*

*Properties can be calculated quickly with a precision of 2 percent or better. Accuracy depends on how well the constants characterizing the intermolecular force law are known; if constants are derived from experimental data, results should be accurate to 5 percent or better. Force constants for 65 gases are tabulated.*

### INTRODUCTION

The kinetic theory of gases has been developed to the point where it is now possible to calculate rather accurately the transport properties of many nonpolar gases and gas mixtures at low pressures (ref. 1). The fundamental equations of rigorous kinetic theory were established by Maxwell and Boltzmann starting nearly a century ago, and in 1916-17 Chapman and Enskog independently obtained general solutions of these equations for the transport properties (ref. 2). However, it is only relatively recently that the necessary transport integrals (which must be evaluated numeri-

cally) have been computed for intermolecular potentials approximating the forces between real molecules (refs. 3 and 4).

The rigorous formula that describes the viscosity of gas mixtures is cumbersome; however, Wilke (ref. 5) has developed an approximate formula, which works rather well. Since Wilke's approximation can be derived from the rigorous expression (ref. 6), it may be used with confidence. A similar approximation has been derived for the thermal conductivity of a mixture of monatomic gases (refs. 6 and 7). It can be used in conjunction with Hirschfelder's expression (ref. 8) for internal energy transport in mixtures to calculate the conductivity of polyatomic gas mixtures.

This paper presents alignment charts designed to permit rapid and accurate calculations according to these equations. The properties are calculable with a precision of 2 percent or better.

The charts for pure gas properties and the binary diffusion coefficients are based on collision integrals for the Lennard-Jones (12-6) potential (ref. 3), which describes the properties of many gases very well. For this potential two parameters are required to specify a molecule's behavior. More elaborate potentials involving three parameters improve agreement with experimental data only slightly (ref. 9).

While the accuracy of the viscosities and conductivities computed for high temperatures may be poor, rigorous calculation of these properties is nonetheless often justified, since in many engineering heat-transfer correlations systematic errors in viscosity and conductivity tend to cancel (ref. 7).

The methods of this paper deal only with the properties of nonpolar gases at low pressures. For gases at high densities or for liquids, the recent text of Reid and Sherwood (ref. 10) is useful. These authors have critically reviewed both theoretical and empirical methods for estimating transport and other properties; they make recommendations as to preferred procedures.

The following two sections discuss the charts for the properties of pure gases and gas mixtures, respectively. The equations that form the basis of the charts are presented and referenced. Examples of their use are presented.

If these charts are to be used extensively, a clear plastic straightedge with a straight line engraved on the back is an extremely useful tool. This device permits rapid and accurate reading and interpolation without marking the charts and without incurring parallax errors.

#### SYMBOLS

$C_p/R$	dimensionless heat capacity
$D$	diffusion coefficient, cm <sup>2</sup> /sec
$k$	Boltzmann constant, erg/°K
$M$	molecular weight, g/g-mole
$P$	pressure, atm
$R$	universal gas constant, cal/(mole) (°K), (eq. (7)), or (cm <sup>3</sup> ) (atm)/(mole) (°K), (eq. (12))
$r$	intermolecular distance, Å (angstrom)
$T$	absolute temperature, °K
$V$	molar volume, cm <sup>3</sup> /mole
$x$	mole fraction
$\epsilon$	maximum energy of attraction, ergs (eq. (1))
$\epsilon/k$	temperature characteristic of intermolecular attraction (eq. (3), table I)
$\eta$	viscosity
$\lambda$	thermal conductivity
$\lambda'$	monatomic thermal conductivity
$\lambda''$	internal thermal conductivity
$\sigma$	zero energy collision diameter, Å (eqs. (1) and (2), table I)
$\Phi_{ij}$	coefficient for calculating the viscosity (eq. (13)) and internal thermal conductivity (eq. (19)) of mixtures

$\phi(r)$	intermolecular potential energy (eq. (1))
$\Psi_{ij}$	coefficient for calculating the monatomic thermal conductivity of gas mixtures (eq. (17))
$\Omega^{(1,1)}$	reduced collision integral for diffusion (eqs. (12) and (22))
$\Omega^{(2,2)}$	reduced collision integral for viscosity (eq. (4)) and thermal conductivity (eq. (6))

#### Subscripts:

$b$	boiling point
$c$	critical point
$i, j$	components $i$ and $j$ of a mixture
$m$	melting point
$mix$	entire mixture
$1, 2$	components 1 and 2 of a mixture

#### PROPERTIES OF PURE GASES

The alignment charts for pure gas properties are based on the Lennard-Jones (12-6) potential,

$$\phi(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] \quad (1)$$

which is a spherically symmetrical function describing the potential energy  $\phi$  of a pair of interacting molecules as a function of intermolecular distance  $r$ . This potential is characterized by two parameters:  $\sigma$ , the zero energy collision diameter, and  $\epsilon$ , the maximum energy of attraction. These parameters, together with the molecular weight, are required to calculate the viscosity and self-diffusion coefficients of pure gases. For estimating thermal conductivity, heat capacities are also required.

Values of  $\sigma$ ,  $\epsilon/k$  (where  $k$  is the Boltzmann constant), and molecular weight for a number of species are shown in table I (pp. 4 and 5). Most of these values have been obtained with viscosity data; however, some estimates for unstable species found in dissociated atmospheric or combustion gases are also included.

In the event  $\sigma$  and  $\epsilon/k$  are not available from transport-property measurements, they may be estimated from critical, boiling, or melting point

properties as follows (ref. 1, p. 245):

$$\left. \begin{aligned} \sigma &\cong 0.841 V_c^{1/3} \text{ (angstroms)} \\ &\cong 1.166 V_b^{1/3} \\ &\cong 1.222 V_m^{1/3} \end{aligned} \right\} \quad (2)$$

$$\left. \begin{aligned} \epsilon/k &\cong 0.77 T_c \\ &\cong 1.15 T_b \\ &\cong 1.92 T_m \end{aligned} \right\} \quad (3)$$

Here  $V_c$ ,  $V_b$ ,  $V_m$  are the molar volumes of the gas at the critical point, the liquid at the boiling point, and the solid at the melting point; while  $T_c$ ,  $T_b$ ,  $T_m$  are the corresponding absolute temperatures. Estimates based on critical properties are to be preferred.

Next, the specific equations and charts for calculating the viscosity, thermal conductivity, and self-diffusion coefficients are considered.

#### VISCOSITY

The viscosity of a pure gas may be written (ref. 1, eq. (8.2-18)):

$$\eta \times 10^6 = 26.693 \frac{\sqrt{MT}}{\sigma^2 \Omega^{(2.2)^*}} \quad (4)$$

where  $\eta$  is the viscosity in  $\text{g}/(\text{cm})(\text{sec})$ , or poise. The quantity  $\Omega^{(2.2)^*}$  is a reduced collision integral that is a function of the reduced temperature  $kT/\epsilon$ . Equation (4) may be rearranged

$$\eta \times 10^6 = 26.693 \left[ \frac{1}{\sigma^2} \sqrt{\frac{M\epsilon}{k}} \right] \left[ \frac{\sqrt{kT/\epsilon}}{\Omega^{(2.2)^*}} \right] \quad (5)$$

Thus, the first bracketed quantity in equation (5) is a constant characteristic of the gas, while the second quantity is a function of  $kT/\epsilon$  alone. Bromley and Wilke (ref. 11) first used equation (5) as the basis of an alignment chart for calculating viscosity.

Figure 1 is an alignment chart based on equation (5). The scales for  $\frac{1}{\sigma^2} \sqrt{\frac{M\epsilon}{k}}$  and viscosity are logarithmic. Hence, these scales can be used for values outside the tabulated range by merely multiplying or dividing by the appropriate power of 10. The reduced temperature scale is so arranged that, if it is read on the left, the viscosity

is as read directly; if the reduced temperature scale is read on the right, the viscosity must be multiplied or divided by 10 as shown in the following examples:

(1) Calculate the viscosity of hydrogen at  $27^\circ \text{C}$ . From table I,  $\epsilon/k = 38.0^\circ \text{K}$ ; hence,

$$\frac{kT}{\epsilon} = \frac{27 + 273}{38} = 7.90$$

Also from table I,  $\frac{1}{\sigma^2} \sqrt{\frac{M\epsilon}{k}} = 1.030$ ; this value is

located on the  $\frac{1}{\sigma^2} \sqrt{\frac{M\epsilon}{k}}$  scale. The point 7.9 is set on the left side of the  $kT/\epsilon$  scale. Hence the viscosity is read directly from the chart as

$$\eta = 90.8 \text{ micropoises} = 6.08 \times 10^{-6} \text{ lb-mass/} \\ (\text{sec})(\text{ft})$$

A smoothed experimental value is 89.6 micropoises (ref. 12).

(2) Estimate the viscosity of cadmium vapor at  $893^\circ \text{K}$ . The melting point of cadmium is  $320.9^\circ \text{C}$ . By equation (3),

$$\epsilon/k \cong 1.92(320.9 + 273.2) = 1141^\circ \text{K}$$

The density of the solid at the melting point is  $8.40 \text{ g/cm}^3$ . Since the atomic weight of cadmium is 112.4, the molar volume at the boiling point is  $112.4/8.40 = 13.38 \text{ cm}^3/\text{mole}$ . From equation (2),

$$\sigma = 1.222(13.38)^{1/3} = 2.90 \text{ \AA}$$

and

$$\frac{1}{\sigma^2} \sqrt{\frac{M\epsilon}{k}} = \frac{1}{(2.90)^2} \sqrt{112.4 \times 1141} = 42.6$$

$$\frac{kT}{\epsilon} = \frac{893}{1141} = 0.783$$

To calculate the viscosity, the value 42.6 is located as 4.26 on the  $\frac{1}{\sigma^2} \sqrt{\frac{M\epsilon}{k}}$  scale (thus, the answer must be multiplied by 10). Because the point 0.783 is set on the right side of the  $kT/\epsilon$  scale, the answer must be divided by 10. Therefore,  $\eta = 564 \times (10/10) = 564 \text{ micropoises}$ . (This same viscosity is obtained by estimating from boiling-point properties.) An experimental value is 665 micropoises (ref. 13).

TABLE I.—CONSTANTS FOR TRANSPORT PROPERTY CALCULATIONS

Gas	Reference no.	Molecular weight	$\sigma$ , Å	$\epsilon/k$ , °K ( <sup>a</sup> )	$\frac{1}{\sigma^2} \sqrt{\frac{M\epsilon}{k}}$ (for viscosity)	$\frac{1}{\sigma^2} \sqrt{\frac{M\epsilon}{k}}$ (for conductivity and diffusion)
Monatomic gases						
He	1	4.003	2.576	10.22	0.964	0.2108
Ne	1	20.18	2.858	27.5	2.884	.1429
Ar	12	39.94	3.421	119.5	5.90	.1478
Kr	1	83.8	3.610	190	9.68	.1155
Xe	1	131.3	4.055	229	10.55	.0803
H	7	1.008	2.68	(38.0)	.862	.855
N		14.01	3.1	(91.5)	3.726	.2659
O		16.00	2.90	(100)	4.757	.2972
F		19.00	2.9	(112)	5.49	.2887
Cl		35.46	3.6	(316)	8.17	.2303
Br		79.9	3.9	(451)	12.48	.1562
I		126.9	4.4	(466)	12.56	.0990
Hg	1	200.6	2.898	851	49.19	.2452
Metastable excited states						
Ne*	7	20.18	7.36	(27.5)	0.4349	0.02155
Ar*	7	39.94	8.73	(119.5)	.906	.02270
Xe*	7	131.3	10.6	(229)	1.543	.01175
Diatomic gases						
Air	1	28.97	3.689	84	3.625	0.1251
H <sub>2</sub>	1	2.016	2.915	38.0	1.030	.511
N <sub>2</sub>	12	28.02	3.681	91.5	3.737	.1334
O <sub>2</sub>	12	32.00	3.499	100	4.620	.1444
F <sub>2</sub>	1	38.00	<sup>b</sup> 3.41	112	5.61	.1476
Cl <sub>2</sub>	( <sup>c</sup> )	70.9	4.217	316	8.42	.1187
Br <sub>2</sub>	( <sup>c</sup> )	159.8	4.403	451	13.85	.0867
I <sub>2</sub>	( <sup>c</sup> )	253.8	5.179	466	12.82	.0505
HCl <sup>d</sup>	1	36.47	3.505	360	10.49	.2876
HI	( <sup>c</sup> )	127.9	4.211	289	10.84	.0848
CO	( <sup>c</sup> )	28.01	3.678	94.5	3.803	.1358
NO	( <sup>c</sup> )	30.01	3.481	121	4.973	.1657

<sup>a</sup> Values in parentheses have been taken from the corresponding diatomic molecule or ground state atom.<sup>b</sup>  $\sigma$  is a mean value estimated by considering viscosity, thermal conductivity, critical temperature and pressure, and boiling-point density.<sup>c</sup> Unpublished values obtained by R. A. Svehla, NASA Lewis Research Center, by a least-squares fit of viscosity data.<sup>d</sup> These gases are sufficiently polar that errors will be encountered in calculating properties of mixtures. (Predicted values will be too low.)



TABLE I.—CONCLUDED. CONSTANTS FOR TRANSPORT PROPERTY CALCULATIONS

Gas	Reference no.	Molecular weight	$\sigma$ , Å	$\epsilon/k$ , °K (*)	$\frac{1}{\sigma^2} \sqrt{\frac{M\epsilon}{k}}$ (for viscosity)	$\frac{1}{\sigma^2} \sqrt{\frac{\epsilon}{Mk}}$ (for con- ductivity and diffusion)
Simple polyatomic gases						
CO <sub>2</sub>	12	44.01	3.952	200	6.01	0.1365
N <sub>2</sub> O	1	44.02	3.816	237	7.01	.1593
NO <sub>2</sub>	27	46.01	3.9	230	6.76	.1470
CS <sub>2</sub>	1	76.1	4.438	488	9.78	.1286
SO <sub>2</sub> <sup>d</sup>	1	64.1	4.290	252	6.91	.1077
COS	1	60.1	4.13	335	8.32	.1384
BF <sub>3</sub>	(c)	67.8	4.200	186	6.37	.0939
BCl <sub>3</sub>	(c)	117.2	5.668	201	4.778	.04076
CH <sub>4</sub>	1	16.04	3.796	144	3.335	.2079
CF <sub>4</sub>	(c)	88.0	4.662	134	4.996	.0568
CCl <sub>4</sub>	(c)	153.8	5.973	315	6.17	.04011
SiF <sub>4</sub>	(c)	104.1	4.880	172	5.62	.0540
SF <sub>6</sub>	(c)	146.1	5.128	222	6.85	.04688
Other inorganic gases						
HgBr <sub>2</sub>	1	360.4	5.414	530	14.91	0.04138
HgI <sub>2</sub>		454.4	5.625	698	17.80	.03917
AsH <sub>3</sub>		77.9	4.06	281	8.98	.1152
SnCl <sub>4</sub>		260.5	4.540	1550	30.83	.1183
SnBr <sub>4</sub>		438.4	6.666	465	10.16	.02318
N <sub>2</sub> O <sub>4</sub>	27	92.0	4.74	383	8.36	.0908
Hydrocarbons						
C <sub>2</sub> H <sub>2</sub>	(c)	26.04	4.023	235	4.833	0.1856
C <sub>2</sub> H <sub>4</sub>	(c)	28.05	4.155	227	4.622	.1648
C <sub>2</sub> H <sub>6</sub>	1	30.07	4.418	230	4.261	.1417
C <sub>3</sub> H <sub>8</sub>		44.09	5.061	254	4.132	.0937
n-C <sub>4</sub> H <sub>10</sub>		58.1	4.997	410	6.18	.1064
iso-C <sub>4</sub> H <sub>10</sub>		58.1	5.341	313	4.727	.0814
n-C <sub>5</sub> H <sub>12</sub>		72.2	5.769	345	4.742	.0657
n-C <sub>6</sub> H <sub>14</sub>		86.2	5.909	413	5.40	.0627
n-C <sub>8</sub> H <sub>18</sub>		114.2	7.451	320	3.443	.03015
n-C <sub>9</sub> H <sub>20</sub>		128.2	8.448	240	2.458	.01917
C <sub>6</sub> H <sub>12</sub> (cyclohexane)		84.2	6.093	324	4.449	.0528
C <sub>6</sub> H <sub>6</sub>		78.1	5.270	440	6.67	.0855
Other organic gases						
CH <sub>3</sub> OH <sup>d</sup>	1	32.04	3.585	507	9.92	0.3095
C <sub>2</sub> H <sub>5</sub> OH		46.07	4.455	391	6.76	.1468
CH <sub>3</sub> Cl <sup>d</sup>		50.5	3.375	855	18.24	.3612
CH <sub>2</sub> Cl <sub>2</sub>		84.9	4.759	406	8.20	.0966
CHCl <sub>3</sub>		119.4	5.430	327	6.70	.0561
CCl <sub>2</sub> F <sub>2</sub>	28	120.9	5.110	288	7.15	.0591
C <sub>2</sub> N <sub>2</sub>	1	52.0	4.38	339	6.92	.1331

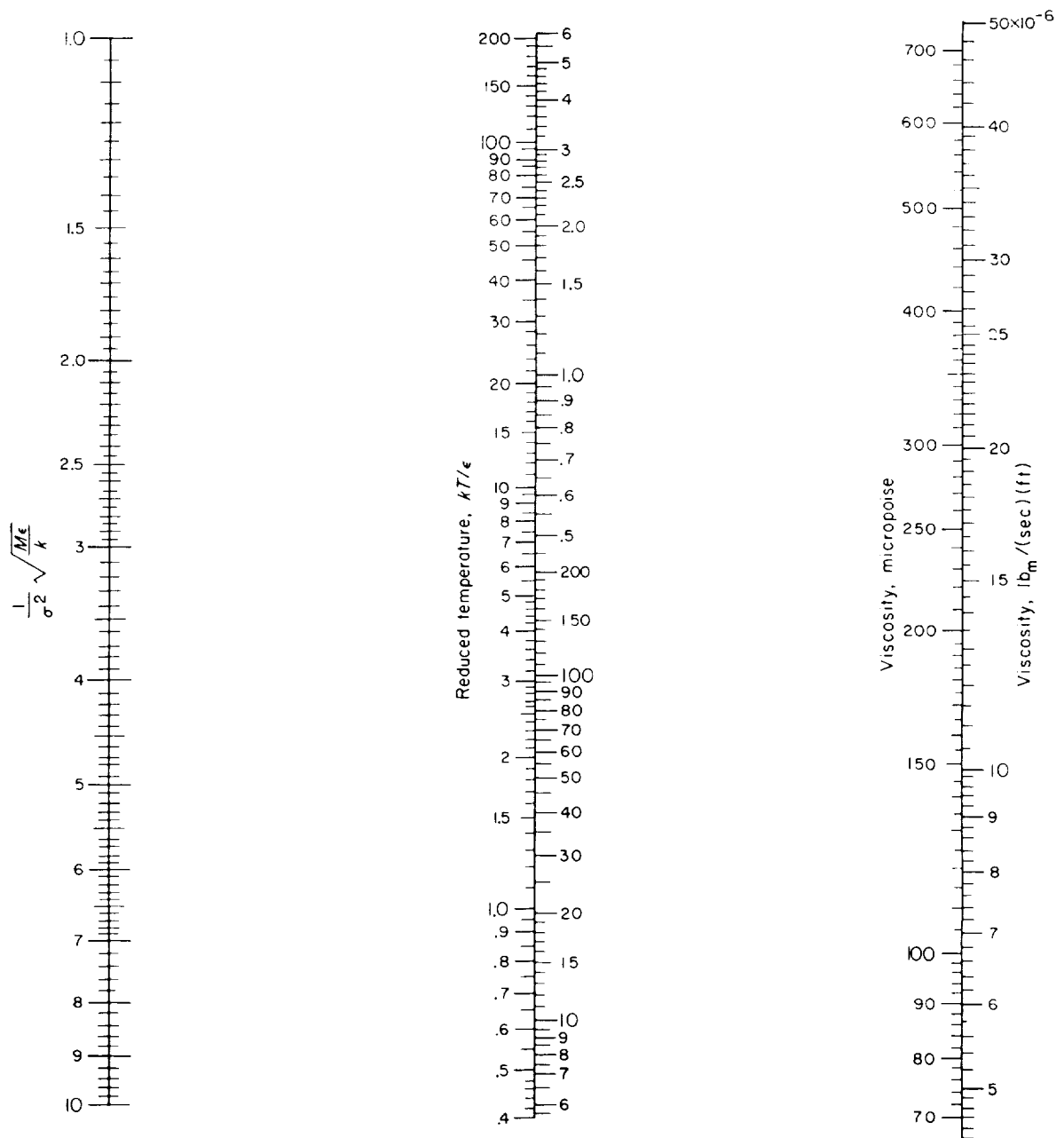


FIGURE 1. Alignment chart for viscosity.

(3) The viscosity of nitrogen at 0° C is 166.2 micropoises (ref. 12). The boiling point of nitrogen is -195.8° C. Estimate the viscosity of nitrogen at (a) 100° K, and (b) 1300° K. From equation (3),

$$\epsilon/k \cong 1.15(273.2 - 195.8) = 89^\circ \text{ K}$$

At 0° C,

$$\frac{kT}{\epsilon} = \frac{273.2}{89} = 3.07$$

From this value and the experimental viscosity,  $\frac{1}{\sigma^2} \sqrt{\frac{M\epsilon}{k}}$  is found to be 3.65. (This value differs somewhat from the value shown in table I because in this example  $\epsilon/k$  was estimated from the boiling point, rather than fitted to viscosity data over a range of temperature; values in table I are to be preferred.) For 100° and 1300° K,  $kT/\epsilon$  values are 1.123 and 14.61. From the chart, the corresponding viscosities are 69.0 and 473 micropoises; values from smoothed experimental data are 68.6 and 466 micropoises (ref. 12).

The errors in these three examples are quite typical. There is close agreement for hydrogen using force constants obtained from experimental viscosity over a range of temperature. Results are almost as good when the critical or boiling point is used to extrapolate from a single experimental measurement over a wide temperature range, as in the nitrogen example just given. Finally, the calculation of the viscosity of cadmium vapor based on melting-point properties was about 15 percent too low. This shows that even in the absence of experimental data reasonable estimates can be made for substances as "unusual" as metal vapors.

#### THEMAL CONDUCTIVITY

The thermal conductivity of a pure monatomic gas is (ref. 1, eq. (8.2-31)):

$$\lambda' \times 10^6 = 198.91 \sqrt{\frac{T/\bar{M}}{\sigma^2 \Omega^{(2,2)}}} \quad (6)$$

$$= \frac{15}{4} \frac{R}{\bar{M}} \eta \times 10^6 \quad (7)$$

where  $\lambda'$  is the monatomic thermal conductivity in cal/(cm)(sec)(°K). In polyatomic gases, addi-

tional heat is conducted through the diffusional transport of internal energy. This contribution to the conductivity  $\lambda''$  is approximated by (ref. 7):

$$\lambda'' \cong 0.88 \left( \frac{2}{5} \frac{C_p}{R} - 1 \right) \lambda' \quad (8)$$

Here  $C_p/R$  is the ratio of the constant-pressure heat capacity to the gas constant. (Heat capacities and specific heats are generally available in handbooks;  $C_p/R$  values for some simple gases are tabulated over a wide range of temperature in ref. 12.) Hence,

$$\lambda = \lambda' \left[ 1 + 0.88 \left( \frac{2}{5} \frac{C_p}{R} - 1 \right) \right] \quad (9)$$

Equation (6) may be rearranged in a fashion analogous to the viscosity expression (eq. (5)) to form the basis of an alignment chart for calculating monatomic thermal conductivity. In this case, the parameter characterizing the gas is  $\frac{1}{\sigma^2} \sqrt{\frac{\epsilon}{Mk}}$ ; values for a number of gases appear in table I.

Figure 2 is an alignment chart for calculating the thermal conductivity of gases based on equations (6) and (9). The  $\frac{1}{\sigma^2} \sqrt{\frac{\epsilon}{Mk}}$ ,  $\frac{kT}{\epsilon}$ , and monatomic conductivity scales are used in a fashion quite analogous to the viscosity chart. If, in calculating the polyatomic conductivity, the  $C_p/R$  scale is read on the right, the answer must be multiplied by 10. If read on the left, the answer is as read from the thermal conductivity scale for  $C_p/R$  from 2.5 to 30; for  $C_p/R$  from 30 to 100, the answer must be multiplied by 100.

The following examples show some uses of figure 2. (As in the case of viscosity, molecular diameters can be estimated from molar volumes. This feature will not be reemphasized.)

(1) Calculate the thermal conductivity of argon at 0° C. From table I,

$$\frac{1}{\sigma^2} \sqrt{\frac{\epsilon}{Mk}} = 0.1478, \quad \frac{\epsilon}{k} = 119.5$$

Hence,

$$\frac{kT}{\epsilon} = \frac{273}{119.5} = 2.28$$

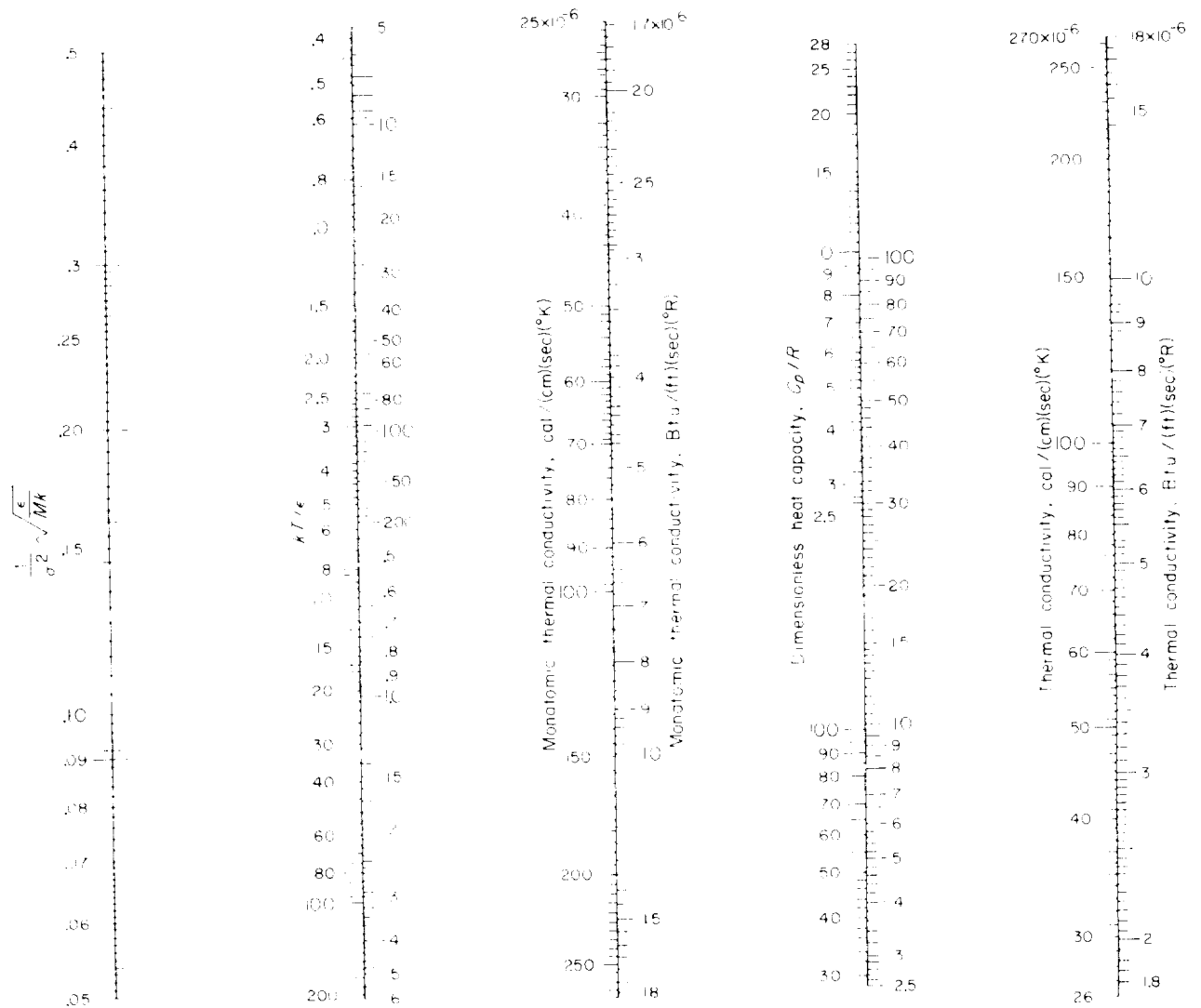


FIGURE 2. Alignment chart for the thermal conductivity.

and, from the chart,

$$\begin{aligned}\lambda' &= 39.2 \times 10^{-6} \text{ cal/(cm) (sec) (}^\circ\text{K)} \\ &= 2.65 \times 10^{-6} \text{ Btu/(ft) (sec) (}^\circ\text{R)}\end{aligned}$$

A smoothed experimental value is  $39.05 \times 10^{-6}$  cal/(cm)(sec)( $^\circ\text{K}$ ) (ref. 12).

(2) Calculate the thermal conductivity of carbon dioxide at  $800^\circ\text{C}$ . From table I,  $\frac{1}{\sigma^2} \sqrt{\frac{\epsilon}{Mk}}$

$= 0.1365$ ,  $\frac{\epsilon}{k} = 200^\circ\text{K}$ , so that

$$\frac{kT}{\epsilon} = \frac{1073}{200} = 5.37$$

From figure 2,

$$\lambda' = 68.8 \times 10^{-6} \text{ cal/(cm) (sec) (}^\circ\text{K)}$$

At  $800^\circ\text{C}$ ,  $C_p/R = 6.63$ ; therefore,

$$\lambda = 169 \times 10^{-6} \text{ cal/(cm) (sec) (}^\circ\text{K)}$$

A value from smoothed experimental data is  $170 \times 10^{-6}$  (ref. 14).

(3) At  $80^\circ\text{C}$  the thermal conductivity of benzene vapor is  $34.8 \times 10^{-6}$  cal/(cm)(sec)( $^\circ\text{K}$ ) (ref. 15). Estimate the thermal conductivity of benzene at  $160^\circ\text{C}$ .

At  $80^\circ\text{C}$  the heat capacity of benzene is 23.6 cal/(deg)(mole), so that  $C_p/R = 11.88$ . From figure 2,

$$\lambda' = \frac{80.6}{10} \times 10^{-6} = 8.06 \times 10^{-6} \text{ cal/(cm) (sec) (}^\circ\text{K)}$$

The boiling point of benzene is  $80.1^\circ\text{C}$ , from which

$$\frac{\epsilon}{k} = 1.15 (273.2 + 80.1) = 406^\circ\text{K}$$

Thus, at  $80^\circ\text{C}$ ,  $kT/\epsilon = 353/406 = 0.869$  and, from figure 2,  $(1/\sigma^2) \sqrt{\epsilon/Mk} = 0.0760$ . Now, for  $160^\circ\text{C}$   $kT/\epsilon = (160 + 273)/406 = 1.067$ . From the chart,

$$\lambda' = 9.90 \times 10^{-6}$$

At  $160^\circ\text{C}$ ,  $C_p = 28.8$  cal/(deg) (mole) and  $C_p/R = 14.5$ . Then

$$\lambda = 52.0 \times 10^{-6} \text{ cal/(cm) (sec) (}^\circ\text{K)}$$

An experimental value is  $54.0 \times 10^{-6}$  cal/(cm) (sec) ( $^\circ\text{K}$ ) (ref. 15).

At a given temperature, the viscosity and thermal conductivity are related through equa-

tions (7) and (9); figure 3 is an alignment chart based on these equations. The scales with the exception of the dimensionless heat-capacity scale are logarithmic and can hence be used for any multiple of 10 of the scale values. The dimensionless heat-capacity scale is identical to that of figure 2. No units are shown, since the chart may be used for several sets of units related as follows:

Viscosity units	Related thermal conductivity units
g/(cm) (sec) or poise	cal/(cm) (sec) ( $^\circ\text{K}$ )
lb <sub>m</sub> /(sec) (ft)	Btu/(ft) (sec) ( $^\circ\text{R}$ )
lb <sub>m</sub> /(hr) (ft)	Btu/(ft) (hr) ( $^\circ\text{R}$ )
lb <sub>m</sub> /(sec) (in.)	Btu/(in.) (sec) ( $^\circ\text{R}$ )
lb <sub>m</sub> /(hr) (in.)	Btu/(in.) (hr) ( $^\circ\text{R}$ )

The use of figure 3 is illustrated by the following examples:

(1) The viscosity of helium at  $0^\circ\text{C}$  is 186.3 micropoises (ref. 16). What is the thermal conductivity of helium? The viscosity of helium is set as 18.6 on the viscosity scale; on this account, the answer must be multiplied by 10. The atomic weight of helium is 4.003; this is set as 40.0 on the molecular weight scale, so that the answer must be multiplied again by 10. From figure 3,

$$\lambda' = 3.48 \times 10^2 \times 10^{-6} = 348 \times 10^{-6} \text{ cal/(cm) (sec) (}^\circ\text{K)}$$

A smoothed experimental value is  $338 \times 10^{-6}$  (ref. 16).

(2) The viscosity of carbon dioxide at  $800^\circ\text{C}$  is 408.0 micropoises (ref. 12). Calculate the thermal conductivity.

The viscosity is set as 40.8, and therefore the answer must be multiplied by 10. Since the molecular weight of carbon dioxide is 44, the monatomic thermal conductivity of carbon dioxide is

$$\begin{aligned}\lambda' &= 6.92 \times 10 \times 10^{-6} \\ &= 69.2 \times 10^{-6} \text{ cal/(cm) (sec) (}^\circ\text{K)}\end{aligned}$$

Since, at  $800^\circ\text{C}$ ,  $C_p/R = 6.63$ ,

$$\lambda = 170 \times 10^{-6} \text{ cal/(cm) (sec) (}^\circ\text{K)}$$

As already noted, a smoothed experimental value is also  $170 \times 10^{-6}$ .

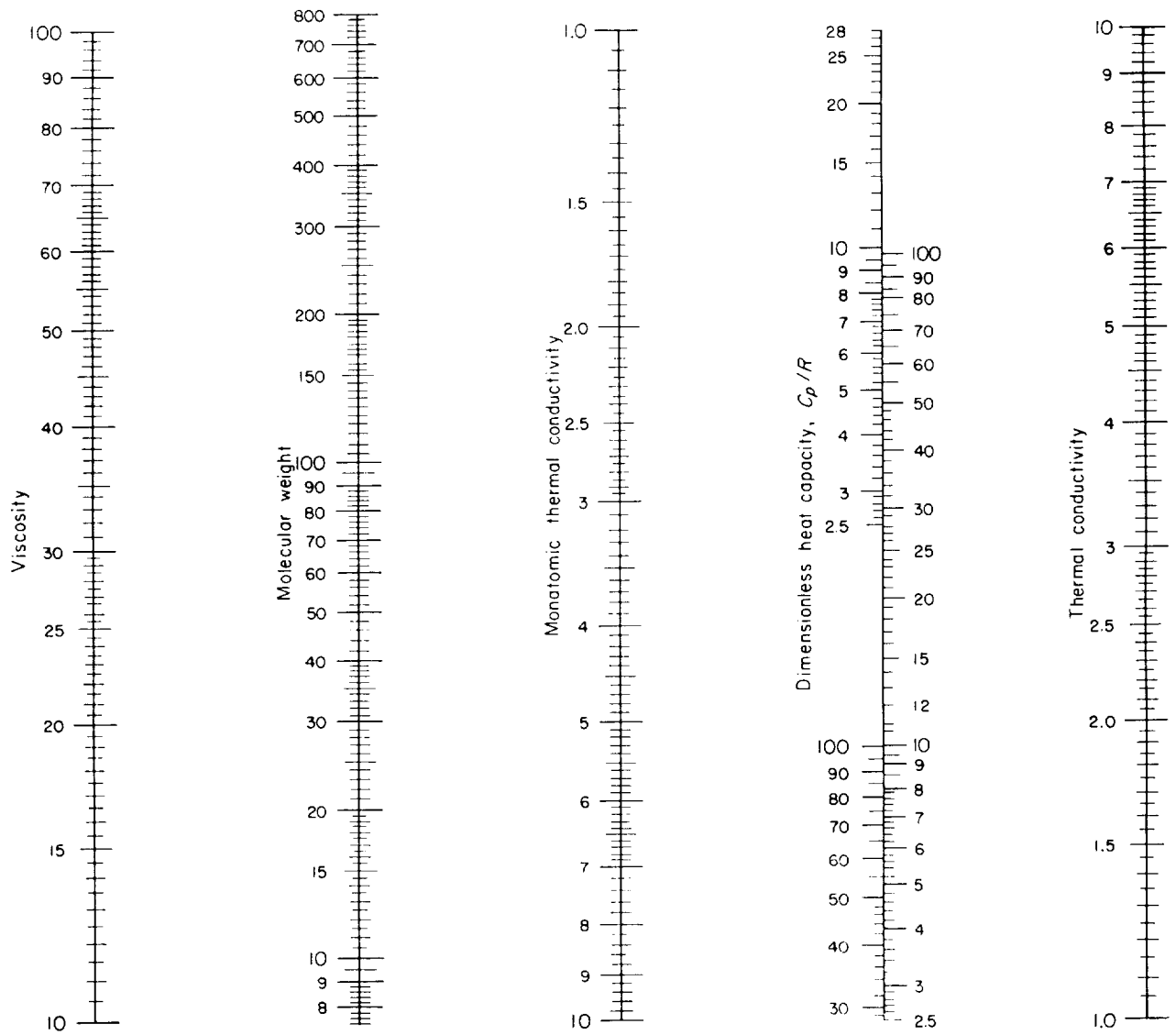


FIGURE 3. -Alignment chart relating viscosity and thermal conductivity.

(3) At 160° C the thermal conductivity of benzene is  $54.0 \times 10^{-6}$  cal/(cm)(sec)(°K) (ref. 15), and the dimensionless heat capacity is 14.5. Estimate the viscosity of benzene. From figure 3,

$$\lambda' = 10.4 \times 10^{-6} \text{ cal/(cm)(sec)(°K)}$$

and, since the molecular weight of benzene is 78.1,

$$\eta = 107 \text{ micropoises}$$

An experimental value is 109.5 micropoises (ref. 15).

The examples calculated with figures 2 and 3 show the results that can be obtained from equations (6), (7), and (9). Equations (6) and (7) are quite reliable, and this is reflected by the rather accurate calculations for the noble gases, argon and helium. The Eucken-type correction embodied in equations (8) and (9) is an approximation that may lead to errors in conductivity on the order of 5 to 10 percent at low temperatures; as the temperature is raised, these errors should decrease. Further, it should be emphasized that these charts will greatly overestimate thermal conductivity for highly polar substances, such as water, ammonia, and methanol (ref. 15).

To calculate the thermal conductivity of polyatomic gas mixtures, it is necessary to know the internal thermal conductivity. (The properties of gas mixtures are treated in the next section.) If an experimental thermal conductivity is available, the internal thermal conductivity may be obtained as the difference between the experimental conductivity and the monatomic conductivity computed from equation (6) or (7), figure 2 or 3:

$$\lambda'' = \lambda - \lambda' \quad (10)$$

In the absence of experimental data, the internal conductivity  $\lambda''$  may be calculated from equation (8). An equivalent procedure is to use the heat capacity to compute the thermal conductivity with figure 2 or 3; the internal conductivity may then be obtained as the difference between the total and monatomic conductivities (eq. (10)).

#### SELF-DIFFUSION COEFFICIENT

The self-diffusion coefficient of a gas, in cm<sup>2</sup>/sec, may be written (ref. 1, eq. (8.2-46)):

$$D = 0.002628 \frac{\sqrt{T^3/M}}{P \sigma^2 \Omega^{(1,1)*}} \quad (11)$$

A different reduced collision integral  $\Omega^{(1,1)*}$  is used in calculating diffusion coefficients. The quotient of the diffusion coefficient and the molar volume  $DP/RT$  is independent of pressure and less markedly dependent on temperature. Thus the equation

$$\frac{DP}{RT} \times 10^6 = 32.03 \left[ \frac{1}{\sigma^2} \sqrt{\frac{\epsilon}{Mk}} \right] \left[ \sqrt{\frac{kT}{\epsilon}} / \Omega^{(1,1)*} \right] \quad (12)$$

forms the basis of the alignment chart for diffusion coefficients shown as figure 4. (In eq. (12) the gas constant  $R$  is in cm<sup>3</sup>/(atm)(deg)(mole).) The parameter  $(1/\sigma^2)\sqrt{\epsilon/Mk}$  characterizes the gas (also used for thermal conductivity). When equation (12) is multiplied by the molecular weight of a gas, the product of diffusion coefficient and density  $\rho D$  is obtained. This quantity often appears in gas dynamic equations.

Actually, the self-diffusion coefficient is not usually an important transport property. The importance of figure 4 lies in the fact that it can be used to calculate binary diffusion coefficients by using properly averaged molecular weight, molecular diameter, and reduced temperature. This is discussed in the section on gas mixtures.

Figure 4 may be used to calculate the self-diffusion coefficient as follows:

(1) Calculate the self-diffusion coefficient of argon at 22° C and 1 atmosphere. From table I,  $\epsilon/k = 119.5$ ,  $(1/\sigma^2)\sqrt{\epsilon/Mk} = 0.1478$ ; hence  $kT/\epsilon = (273.2 + 22)/119.5 = 2.47$ . From figure 4,  $DP/RT = 7.52 \times 10^{-6}$  g-moles/(cm)(sec). Hence,

$$D = (7.52 \times 10^{-6}) \frac{RT}{P} = 7.52 \times 10^{-6} \frac{82.06 \times 295.2}{1} \\ = 0.182 \text{ cm}^2/\text{sec}$$

An experimental value is 0.180 cm<sup>2</sup>/sec (ref. 17).

#### PROPERTIES OF GAS MIXTURES

The charts of the previous section, devoted to calculation of the properties of pure gases, are in the main based on rigorous kinetic theory. The rigorous theory for the viscosity and thermal conductivity of gas mixtures is also well developed (refs. 1 (eq. (8.2-25)), 8, and 18), but the formulas are complex. Simpler approximations, derived from rigorous theory, are presented here. On the other hand, the binary diffusion coefficient equation is exact.

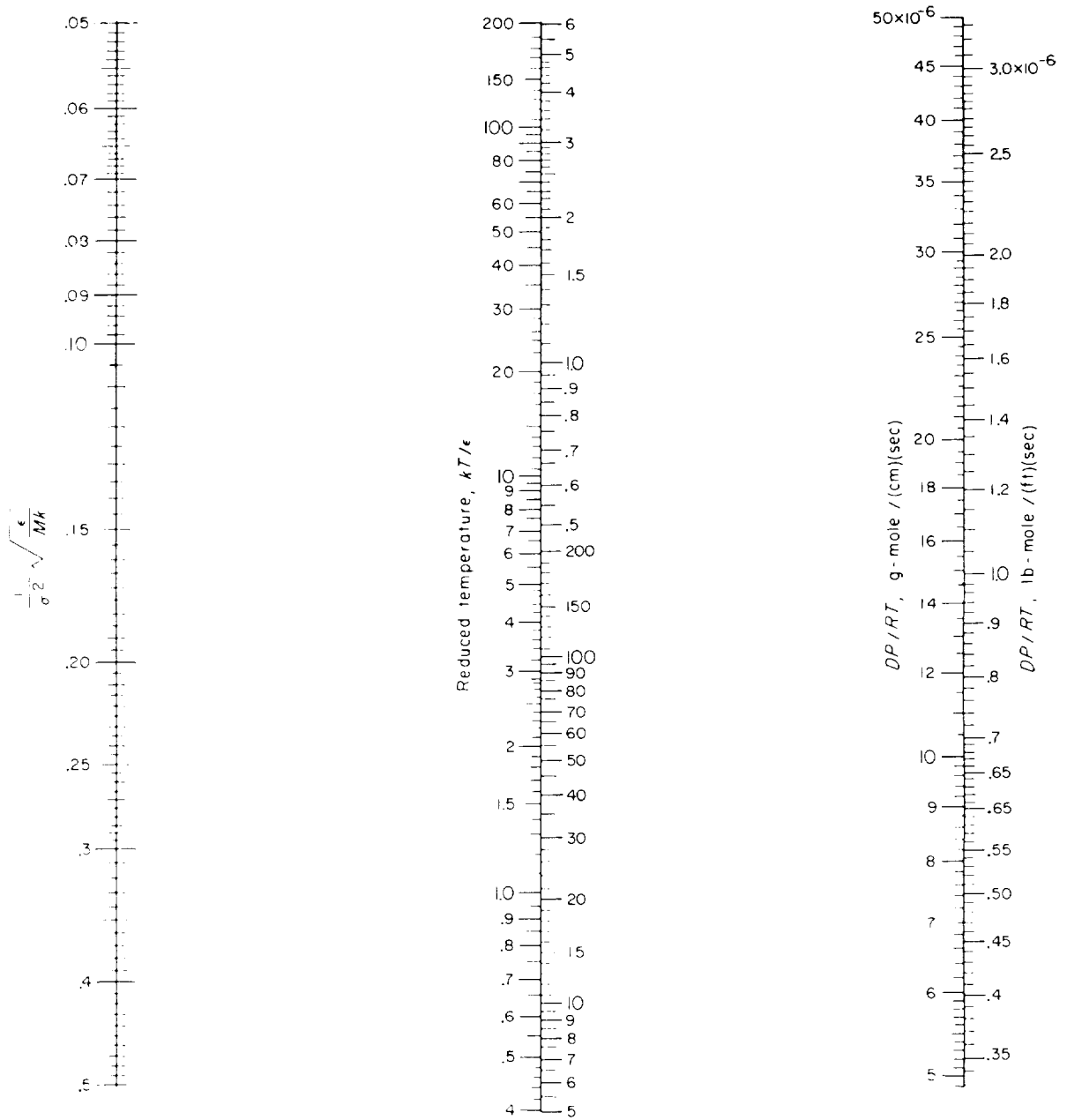


FIGURE 4. Alignment chart for diffusion coefficient.



## VISCOSITY

The viscosity of a gas mixture of  $\nu$  components may be calculated by the approximate equation (ref. 7):

$$\eta_{mix} = \sum_{i=1}^{\nu} \frac{\eta_i}{1 + \sum_{\substack{j=1 \\ j \neq i}}^{\nu} \Phi_{ij} \frac{x_j}{x_i}} \quad (13)$$

where the  $\eta_i$  are the viscosities of the component gases and  $x_i$ ,  $x_j$  are mole fractions. The coefficients  $\Phi_{ij}$  are given as a function of the viscosity and molecular-weight ratios of species  $i$  and  $j$ :

$$\Phi_{ij} = \frac{\left[1 + \left(\frac{\eta_i}{\eta_j}\right)^{1/2} \left(\frac{M_j}{M_i}\right)^{1/4}\right]^2}{2\sqrt{2} \left(1 + \frac{M_i}{M_j}\right)^{1/2}} \quad (14)$$

Equations (13) and (14) were first developed empirically by Wilke (ref. 5); these equations have been related to the rigorous theory in references 6 and 7.

Figures 5 and 6 are charts for calculating  $\Phi_{ij}$  based on equation (14). It is believed that almost all cases can be obtained from figure 5; however, figure 6 is provided for large values of viscosity ratio.

Once  $\Phi_{ij}$  has been obtained from figure 5 or 6,  $\Phi_{ji}$  may be similarly obtained. Alternatively, it may be computed from the equation

$$\Phi_{ji} = \Phi_{ij} \left( \frac{\eta_j}{\eta_i} \right) \left( \frac{M_i}{M_j} \right) \quad (15)$$

The following example illustrates the use of figure 5 or 6 and equations (13) and (15):

(1) At 23° C the viscosities of hydrogen and carbon dioxide are 89.1 and 149.3 micropoises, respectively, (values cited in ref. 19). What is the viscosity of a mixture of 41.3 percent hydrogen in carbon dioxide?

Designating hydrogen as species 1 and carbon dioxide as species 2,  $\eta_1/\eta_2=0.596$  and  $M_1/M_2=0.0458$ . From figure 5,  $\Phi_{12}=2.46$ . Similarly,  $\eta_2/\eta_1=1.676$  and  $M_2/M_1=21.82$ ; and from figure 5  $\Phi_{21}=0.191$ . (Alternatively, from eq. (15)  $\Phi_{21}=2.46 \times 1.676 \times 0.0458=0.1888$ .) Hence, from equation (13),

$$\eta_{mix} = \frac{89.1}{1 + 2.46 \frac{0.413}{0.413}} + \frac{149.3}{1 + 0.191 \frac{0.413}{1-0.413}} = 151.6 \text{ micropoises}$$

This is in excellent agreement with both the experimental viscosity of 150.6 micropoises (cited in ref. 19) and the rigorously calculated viscosity, 150.8 micropoises (ref. 19).

Comparisons of viscosities from equations (13) and (14) with rigorously calculated mixture viscosities suggest that the approximate formulas have a probable error of about 2 percent (ref. 7).

## THERMAL CONDUCTIVITY

The thermal conductivity of a mixture of polyatomic gases may be divided into two portions:

$$\lambda_{mix} = \lambda'_{mix} + \lambda''_{mix} \quad (16)$$

Here  $\lambda'_{mix}$  represents the monatomic thermal conductivity of the mixture, whereas  $\lambda''_{mix}$  accounts for the diffusional transport of internal energy.

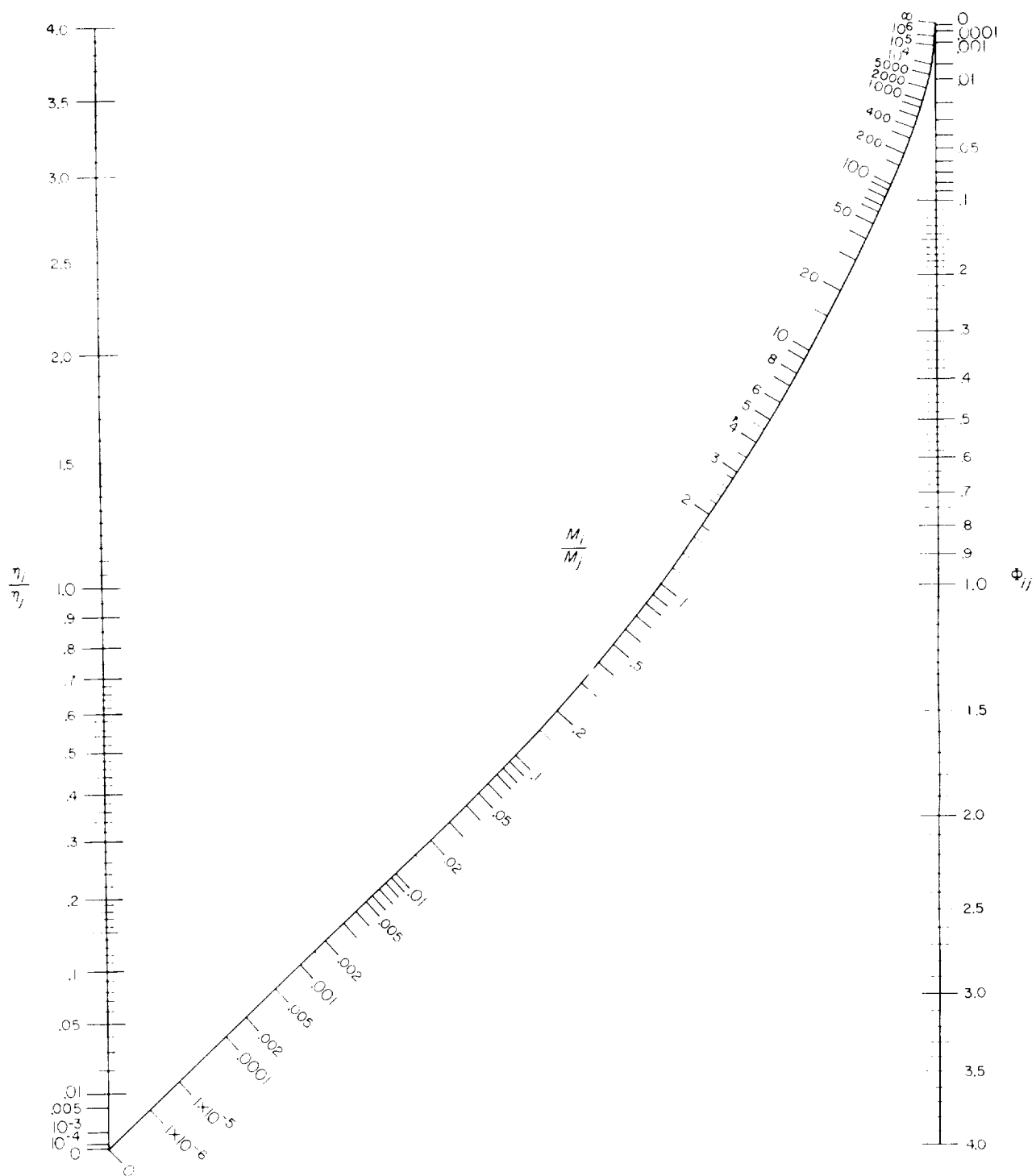
The approximate formula for the monatomic mixture conductivity is (ref. 6):

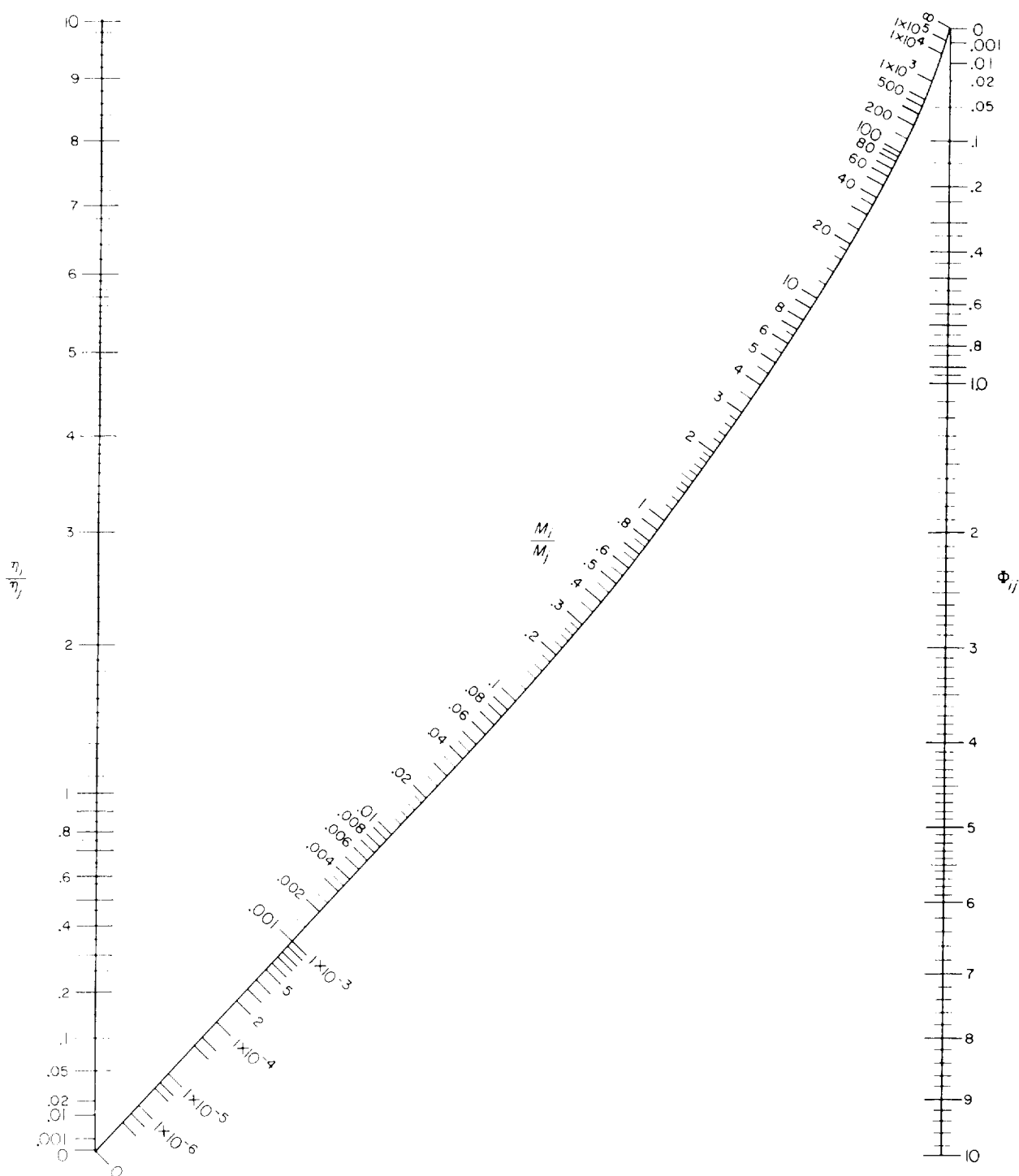
$$\lambda'_{mix} = \sum_{i=1}^{\nu} \frac{\lambda'_i}{1 + \sum_{\substack{j=1 \\ j \neq i}}^{\nu} \Psi_{ij} \frac{x_j}{x_i}} \quad (17)$$

where the  $\lambda'_i$  are the monatomic thermal conductivities of the pure component gases. The coefficients  $\Psi_{ij}$  are found to be (ref. 7):

$$\begin{aligned} \Psi_{ij} &= \Phi_{ij} \left[ 1 + 2.41 \frac{(M_i - M_j)(M_i - 0.142 M_j)}{(M_i + M_j)^2} \right] \\ &= \frac{\left[ 1 + \left( \frac{\lambda'_i}{\lambda'_j} \right)^{1/2} \left( \frac{M_j}{M_i} \right)^{1/4} \right]^2}{2\sqrt{2} \left( 1 + \frac{M_i}{M_j} \right)^{1/2}} \\ &\quad \left[ 1 + 2.41 \frac{(M_i - M_j)(M_i - 0.142 M_j)}{(M_i + M_j)^2} \right] \quad (18) \end{aligned}$$

Figures 7 and 8 are charts for calculating  $\Psi_{ij}$  as a function of the monatomic conductivity and molecular weight ratios; figure 7 is for small  $\Psi_{ij}$  and figure 8 is for large values. It should be noted that there is no simple form analogous to equation (15) relating  $\Psi_{ij}$  and  $\Psi_{ji}$ .

FIGURE 5. -Alignment chart for  $\phi_{ij}$  from viscosity.

FIGURE 6.—Alignment chart for  $\Phi_{ij}$  from viscosity (large values of  $\Phi_{ij}$  and viscosity ratio).

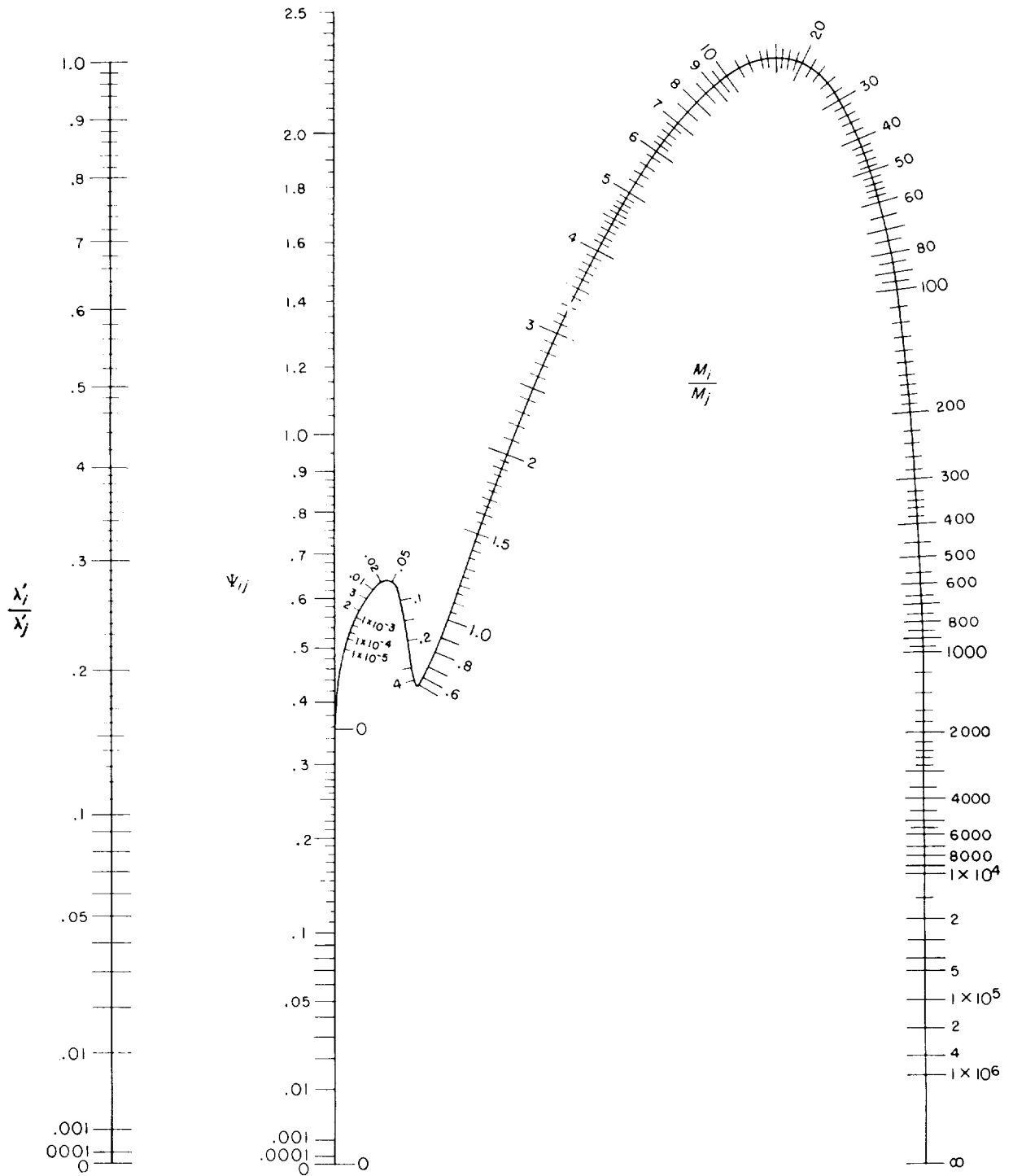


FIGURE 7. Alignment chart for  $\Psi_{ij}$  from conductivity (small values of  $\Psi_{ij}$  and monatomic conductivity ratio).

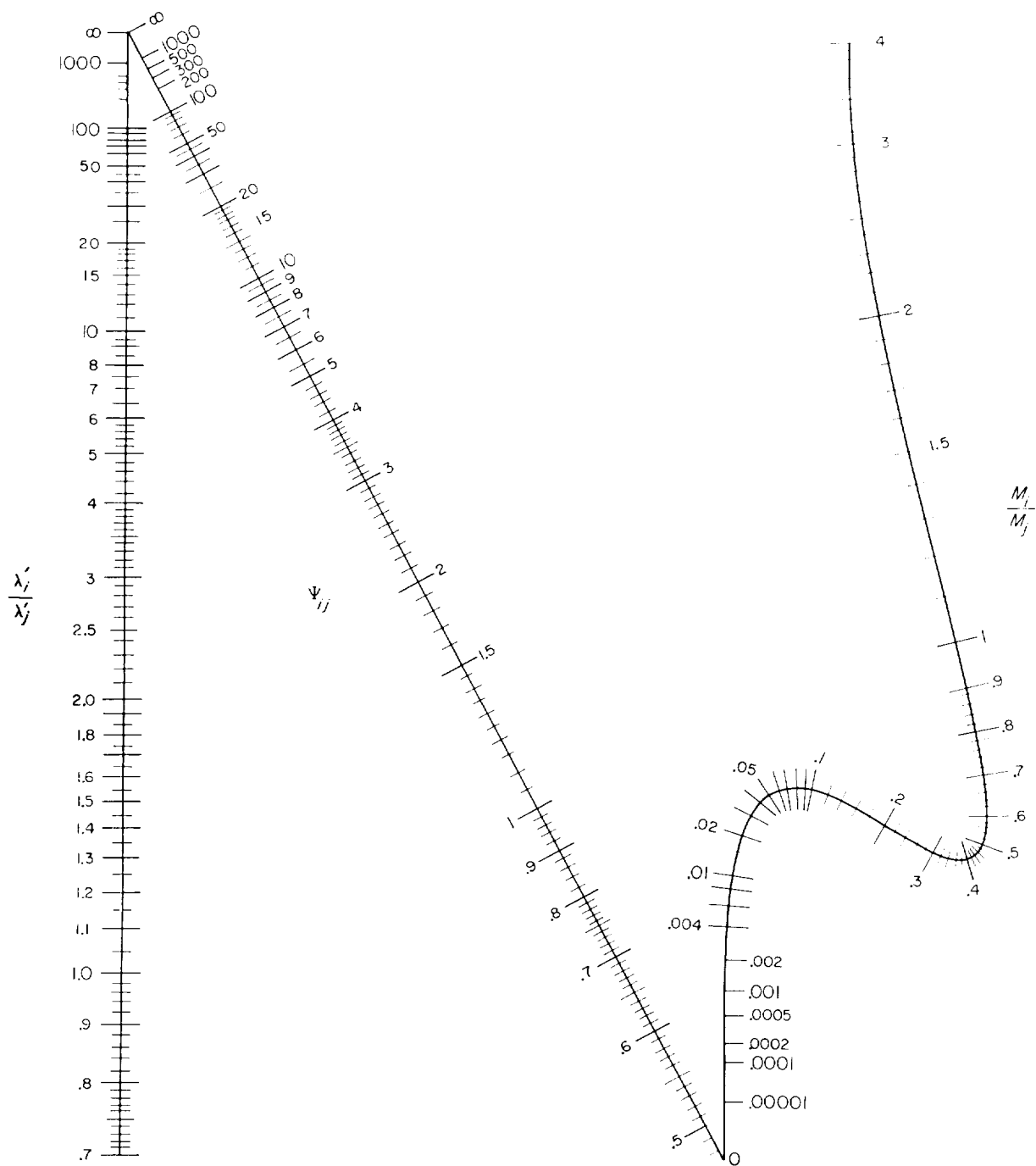


FIGURE 8.—Alignment chart for  $\Psi_{ij}$  from conductivity (large values of  $\Psi_{ij}$  and monatomic conductivity ratio).

The following example illustrates the use of figures 7 and 8 together with equation (17):

(1) At 311° K the thermal conductivities of helium, argon, and xenon are 375.3, 43.8, and  $13.5 \times 10^{-6}$  cal/(cm) (sec) (°K), respectively (ref. 20). What is the thermal conductivity of a mixture of 39.01 percent helium, 36.75 percent argon, and 24.24 percent xenon?

Details of the calculation are presented in tabular form below.

Equation (17) becomes

$$\begin{aligned}\lambda'_{mix} &= \frac{375.3}{1 + 2.41 + 2.73} + \frac{43.8}{1 + 0.805 + 0.937} \\ &\quad + \frac{13.5}{1 + 0.656 + 1.522} \\ &= 81.3 \times 10^{-6} \text{ cal/(cm) (sec) (°K)}\end{aligned}$$

A value of  $84.5 \times 10^{-6}$  cal/(cm) (sec) (°K) is found for this mixture both experimentally (ref. 20) and from rigorous theory (ref. 18).

A formula for  $\lambda''_{mix}$ , the internal thermal conductivity, has been derived by Hirschfelder (ref. 8). This expression, which embodies a treatment of the diffusional transport of internal energy, can be approximated by an expression analogous to equation (13) (ref. 7):

$$\lambda''_{mix} = \sum_{i=1}^p \frac{\lambda''_i}{1 + \sum_{\substack{j=1 \\ j \neq i}}^p \Phi_{ij} \frac{x_j}{x_i}} \quad (19)$$

where the  $\lambda''_i$  are the internal thermal conductivities of the pure component gases. If experimental conductivities for the pure gases are known, the  $\lambda''_i$  are best obtained as the difference between

experimental and monatomic conductivities (eq. (10)). The coefficient  $\Phi_{ij}$  (the same coefficient required for mixture viscosity) can be expressed as a function of monatomic thermal conductivity and molecular weight ratios (ref. 7).

$$\Phi_{ij} = \frac{\left[1 + \left(\frac{\lambda'_i}{\lambda'_j}\right)^{1/2} \left(\frac{M_i}{M_j}\right)^{1/4}\right]^2}{2\sqrt{2} \left(1 + \frac{M_i}{M_j}\right)^{1/2}} \quad (20)$$

Figures 9 and 10 are charts based on equation (20) (fig. 9 for small  $\Phi_{ij}$ , fig. 10 for large  $\Phi_{ij}$ ). The coefficients  $\Phi_{ij}$  and  $\Phi_{ji}$  are related:

$$\Phi_{ji} = \Phi_{ij} \frac{\lambda'_j}{\lambda'_i} \quad (21)$$

The use of these relations is illustrated by the following examples:

(1) At 0° C the  $C_p/R$  for hydrogen and carbon dioxide are 3.44 and 4.32, respectively. What is the thermal conductivity of a 50 percent mixture of hydrogen in carbon dioxide?

From figure 2, together with the constants in table 1, the monatomic thermal conductivities  $\lambda'$  of hydrogen and carbon dioxide are  $312 \times 10^{-6}$  and  $22.8 \times 10^{-6}$  cal/(cm) (sec) (°K), respectively. With hydrogen designated as species 1 and carbon dioxide as species 2,  $\lambda'_1/\lambda'_2 = 13.68$ ,  $M_1/M_2 = 0.0458$ ; and  $\lambda'_2/\lambda'_1 = 0.0731$ ,  $M_2/M_1 = 21.82$ . From figures 7 and 8,  $\Psi_{12} = 3.05$  and  $\Psi_{21} = 0.570$ . From equation (17) the monatomic thermal conductivity is

$$\begin{aligned}\lambda'_{mix} &= \frac{312}{1 + 3.05 \frac{0.5}{0.5}} + \frac{22.8}{1 + 0.570 \frac{0.5}{0.5}} \\ &= 91.6 \times 10^{-6} \text{ cal/(cm) (sec) (°K)}\end{aligned}$$

Component		$\lambda'_i/\lambda'_j$	$M_i/M_j$	$\Phi_{ij}$ (figs. 7 and 8)	$x_j/x_i$	$\Psi_{ij} \frac{x_j}{x_i}$
$i$	$j$					
He	Ar	8.57	0.1002	2.56	0.941	2.41
	Xe	27.8	.03045	4.49	.621	2.73
Ar	He	.1167	9.98	.757	1.062	.805
	Xe	3.24	.304	1.42	.660	.937
Xe	He	.03596	32.80	.408	1.609	.656
	Ar	.308	3.288	1.005	1.514	1.522

From figure 2, together with the dimensionless heat capacities, the conductivities are found to be  $\lambda_1 = 416 \times 10^{-6}$ ,  $\lambda_2 = 37.3 \times 10^{-6}$ . Then from equation (10)  $\lambda_1'' = 104 \times 10^{-6}$ ,  $\lambda_2'' = 14.5 \times 10^{-6}$  cal/(cm) (sec) ( $^{\circ}\text{K}$ ). From figure 10,  $\Phi_{12} = 2.53$  and, from figure 9,  $\Phi_{21} = 0.186$  (from eq. (21)  $\Phi_{21} = 2.53 \times 0.0731 = 0.185$ ). From equation (19) the internal thermal conductivity is

$$\lambda_{mix}'' = \frac{104}{1 + 2.53 \frac{0.5}{0.5}} + \frac{14.5}{1 + 0.186 \frac{0.5}{0.5}}$$

$$= 41.7 \times 10^{-6} \text{ cal/(cm) (sec) } (^{\circ}\text{K})$$

By equation (16)  $\lambda_{mix} = (91.6 + 41.7) \times 10^{-6} = 133.3 \times 10^{-6}$  cal/(cm) (sec) ( $^{\circ}\text{K}$ ). An experimental measurement for this mixture gives a conductivity  $135 \times 10^{-6}$  cal/(cm) (sec) ( $^{\circ}\text{K}$ ) (ref. 21).

(2) At  $0^{\circ}\text{C}$  the thermal conductivities of hydrogen and carbon dioxide are  $404 \times 10^{-6}$  and  $36 \times 10^{-6}$  cal/(cm) (sec) ( $^{\circ}\text{K}$ ), respectively. Calculate the thermal conductivity of a 50 percent mixture of hydrogen in carbon dioxide.

In this case, the monatomic thermal conductivities of the pure gases and the mixture are obtained exactly as in the preceding example; the internal thermal conductivities, however, are obtained from equation (10) with the experimental conductivities:

$$\lambda_1'' = (404 - 312) \times 10^{-6} = 92 \times 10^{-6} \text{ cal/(cm) (sec) } (^{\circ}\text{K})$$

$$\lambda_2'' = (36 - 22.8) \times 10^{-6} = 13.2 \times 10^{-6}$$

The internal conductivity is

$$\lambda_{mix}'' = \frac{92}{1 + 2.53} + \frac{13.2}{1 + 0.186}$$

$$= 37.2 \times 10^{-6} \text{ cal/(cm) (sec) } (^{\circ}\text{K})$$

and from equation (16)  $\lambda_{mix} = (91.6 + 37.2) \times 10^{-6} = 128.8 \times 10^{-6}$  cal/(cm) (sec) ( $^{\circ}\text{K}$ ). As noted in the previous example, the experimental value is  $135 \times 10^{-6}$  cal/(cm) (sec) ( $^{\circ}\text{K}$ ). A value computed by using rigorous formulas is  $135.0 \times 10^{-6}$  cal/(cm) (sec) ( $^{\circ}\text{K}$ ) (ref. 8).

In general, the procedure used in the second example is to be preferred—that is to say, it is best to estimate the internal conductivities of the pure components from their thermal conductivities

(when available) rather than their heat capacities. (The fact that this procedure gives poorer agreement with experiment in this example is fortuitous.)

Comparisons of calculations using these approximate mixture thermal-conductivity equations with rigorously computed mixture conductivities suggest that these approximations have a probable error of about 1.5 percent (ref. 7).

Finally, it should be noted that in chemically reacting gas mixtures there may be a very large increase in thermal conductivity due to the diffusional transport of chemical enthalpy. A general expression has been derived for the increase in thermal conductivity due to chemical reactions in gas mixtures at chemical equilibrium (refs. 22 and 23); this effect can account under some conditions for an eightfold increase in the thermal conductivity of nitrogen tetroxide vapor (refs. 7 and 24) and a thirtyfold increase in the conductivity of hydrogen fluoride vapor (refs. 7 and 25). In order to compute the increase in thermal conductivity due to reaction, the gas composition, heats of reaction, and binary diffusion coefficients among the component gases are required. The next section deals with the calculation of binary diffusion coefficients.

#### BINARY DIFFUSION COEFFICIENT

The binary diffusion between two gases may be written (ref. 1, eq. (8.2-44)):

$$D_{12} = 0.002628 \sqrt{\frac{T^3(M_1 + M_2)/2M_1M_2}{P\sigma_{12}^2\Omega_{12}^{(1,1)*}}} \quad (22)$$

Here  $D_{12}$  is the binary diffusion coefficient between species 1 and 2,  $M_1$  and  $M_2$  are the molecular weights, and  $\sigma_{12}$  is a collision diameter characteristic of the unlike molecule interaction. In this case, the reduced collision integral  $\Omega_{12}^{(1,1)*}$  is a function of a reduced temperature  $kT/\epsilon_{12}$ .

The parameters  $\epsilon_{12}/k$  and  $\sigma_{12}$  may be approximated as the geometric and arithmetic means, respectively,

$$\epsilon_{12}/k = [(\epsilon_1/k)(\epsilon_2/k)]^{1/2} \quad (23)$$

$$\sigma_{12} = \frac{1}{2}(\sigma_1 + \sigma_2) \quad (24)$$

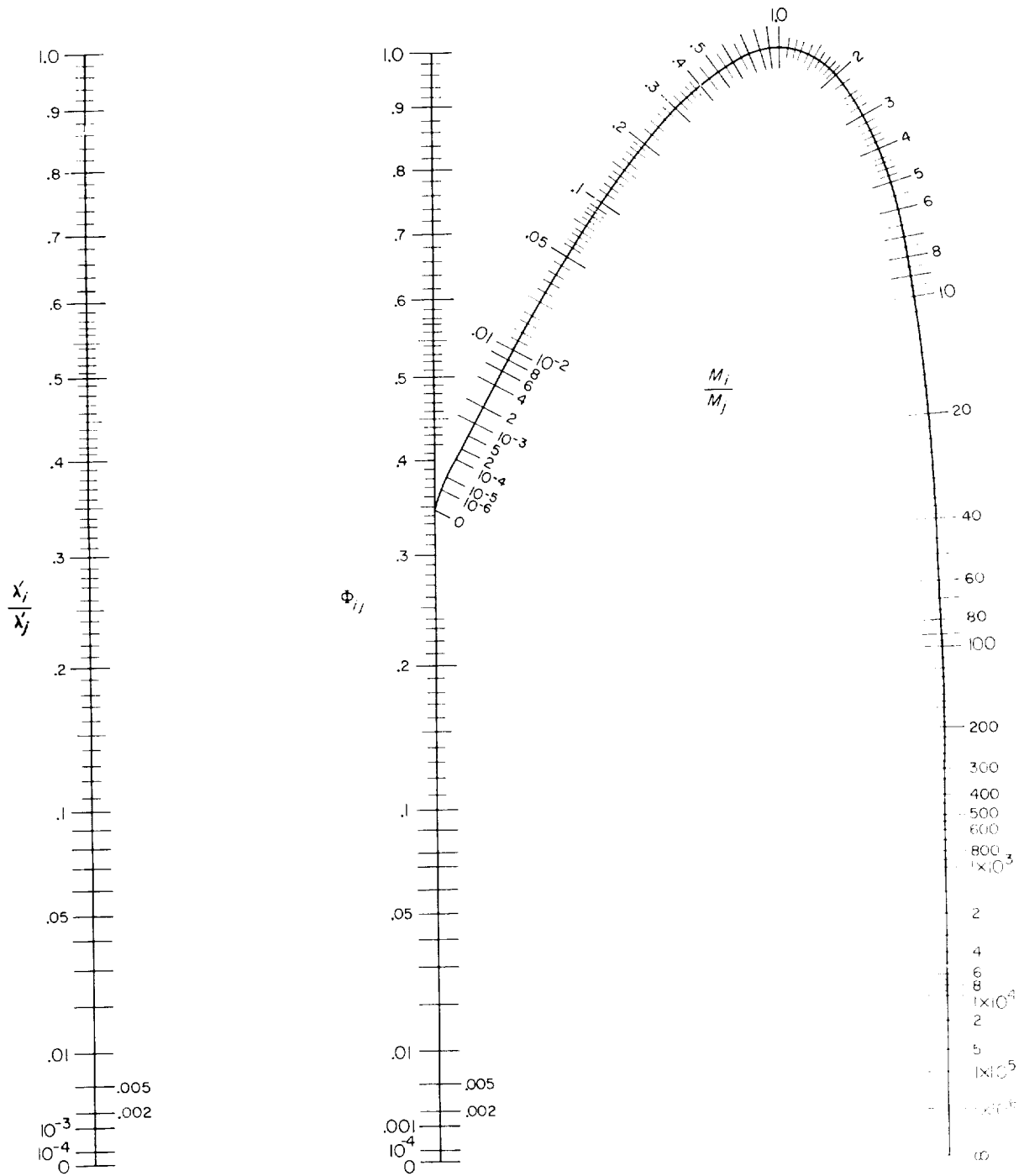


FIGURE 9.—Alignment chart for  $\Phi_{ij}$  from conductivity (small values of  $\Phi_{ij}$  and monatomic conductivity ratio).



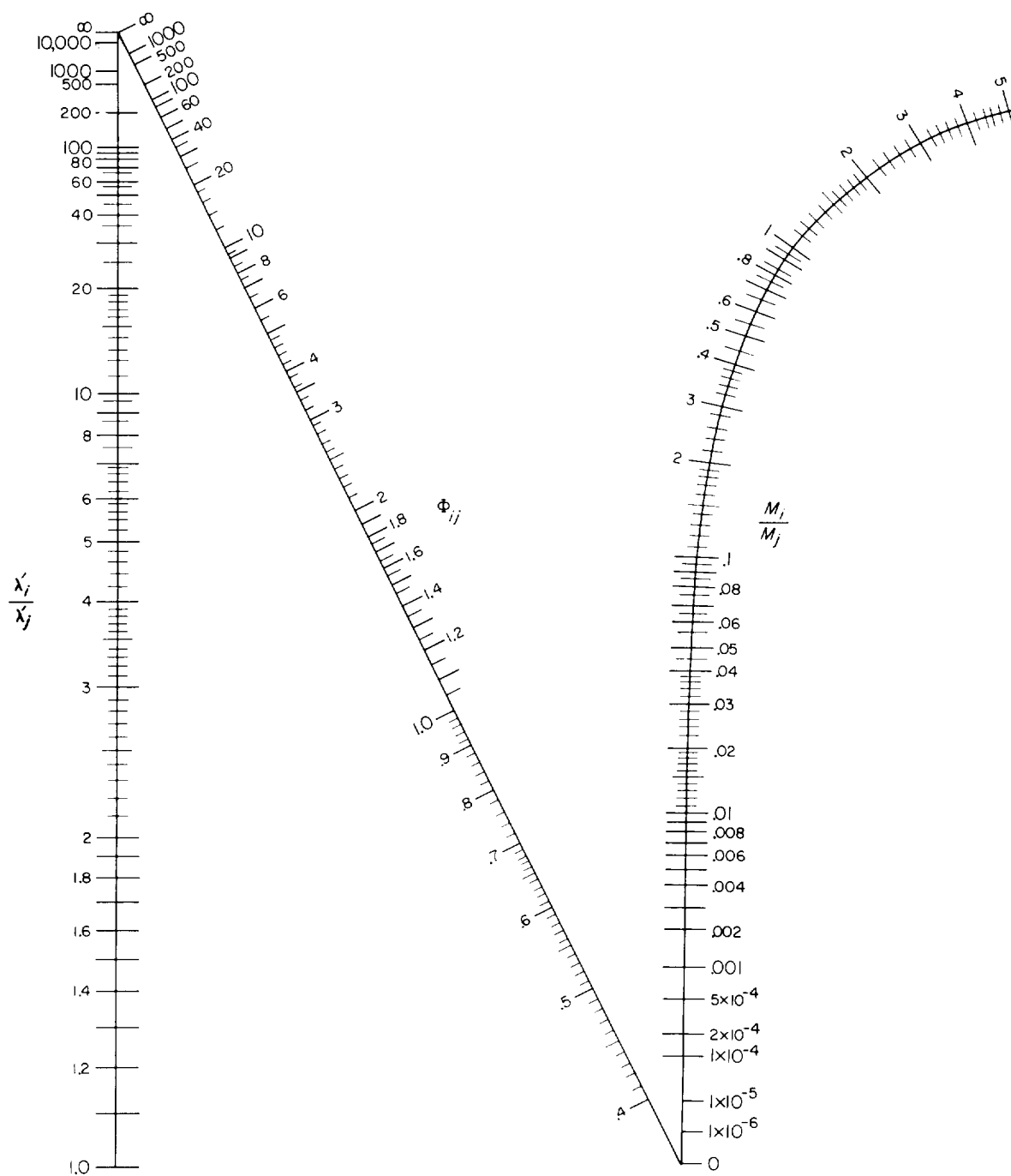


FIGURE 10. Alignment chart for  $\Phi_{ij}$  from conductivity (large values of  $\Phi_{ij}$  and monatomic conductivity ratio).

In addition, a reciprocal average molecular weight can be defined:

$$\frac{1}{M_{12}} = \frac{1}{2} \left( \frac{1}{M_1} + \frac{1}{M_2} \right) \quad (25)$$

Then the quotient of the binary diffusion coefficient and the molar volume is given by equation (12) and figure 4, with  $\epsilon$ ,  $\sigma$ , and  $M$  average values calculated from equations (23) to (25).

The following example illustrates the use of figure 4 and equations (23) to (25) in calculating binary diffusion coefficients:

(1) Calculate the hydrogen-nitrogen diffusion coefficient at 85° C and 1 atmosphere.

From the force constants from table I, together with equations (23) to (25),  $\sigma_{12} = 3.298$ ,  $\epsilon_{12}/k = 59^\circ$  K,  $M_{12} = 3.76$ , and  $(1/\sigma^2) \sqrt{\epsilon/Mk} = 0.364$ . Therefore,

$$\frac{kT}{\epsilon} = \frac{85 + 273.2}{59} = 6.07$$

From figure 4,  $DP/RT = 36.0 \times 10^{-6}$  g-mole/(cm) (sec). Hence,

$$D_{12} = 36.0 \times 10^{-6} \frac{RT}{P} = 36.0 \times 10^{-6} \times \frac{82.06 \times 358.2}{1} = 1.058 \text{ cm}^2/\text{sec}$$

An experimental value is 1.052 cm<sup>2</sup>/sec (ref. 26).

## CONCLUDING REMARKS

The alignment charts presented in this report are believed to represent the best general methods now available for computing the transport properties of pure nonpolar gases based on rigorous kinetic theory. On the other hand, although the binary diffusion coefficient calculations are rigorous, the formulas used for mixture viscosity and conductivity are approximations based on rigorous theory. They are believed to be accurate enough for all practical applications. However, they are not suitable for comparing experimental data with theory; for this purpose, rigorous calculations should be made.

Although these charts are not applicable to highly polar gases, they can probably be used for order-of-magnitude estimates. The mixture formulas should give approximately correct results for mixtures with traces of polar constituents.

The sole exception is the binary diffusion coefficient chart. This should be suitable for calculating diffusion coefficients between polar and nonpolar gases, provided the force constants  $\sigma_{12}$  and  $\epsilon_{12}/k$  are properly chosen.

LEWIS RESEARCH CENTER

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION  
CLEVELAND, OHIO, May 27, 1960

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